SYLLABUS

1. Information regarding the programme

1.1 Higher education institution	**Babeş-Bolyai University**
1.2 Faculty	**Physics**
1.3 Department	**Physics**
1.4 Field of study	**Physics**
1.5 Study cycle	**Master**
1.6 Study programme / Qualification	**Computational physics**

2. Information regarding the discipline

2.1 Name of the discipline	**Numerical computations in atomic physics**						
2.2 Course coordinator	**Ladislau Nagy**						
2.3 Seminar coordinator	**Sándor Borbély**						
2.4. Year of study	1	2.5 Semester	2	2.6. Type of evaluation	E	2.7 Type of discipline	Speciality

3. Total estimated time (hours/semester of didactic activities)

3.1 Hours per week	4	Of which: 3.2 course	2	3.3 seminar/laboratory	2
3.4 Total hours in the curriculum	56	Of which: 3.5 course	28	3.6 seminar/laboratory	28
Time allotment:					hours
Learning using manual, course support, bibliography, course notes					22
Additional documentation (in libraries, on electronic platforms, field documentation)					20
Preparation for seminars/labs, homework, papers, portfolios and essays					32
Tutorship					10
Evaluations					
Other activities:					

3.7 Total individual study hours	84
3.8 Total hours per semester	140
3.9 Number of ECTS credits	6

4. Prerequisites (if necessary)

4.1. curriculum	
4.2. competencies	• quantum mechanics, atomic physics, numerical methods, programming in C (or Fortran) and Python

5. Conditions (if necessary)

5.1. for the course	•
5.2. for the seminar /lab activities	•

6. Specific competencies acquired

Specific competences	• **Using in-depth knowledge of physics, mathematics, and programming in various multi- and inter-disciplinary fields.** • **Applying atomic physics to understand of complex scientific phenomena.** • **Making effective use of in-depth knowledge of physics, mathematics in solving real problems in atomic physics** • **Using advanced information technology and electronic communication in order to analyze, model, simulate, and aggregate data from various branches of physics or other related fields.** • **Solving advanced problems of atomic physics by means of field-related mathematical and computer instruments (analytical, numerical, or statistical tools).** • **Communicating complex scientific ideas, experiments or outcomes of a scientific project.** • **Efficient use of high-performance computing infrastructure for solving atomic physics problems.**
Transversal competences	• **Accomplishment of professional tasks in an effective and responsible manner, in compliance with the field-specific legislation and code of ethics.** • **Implementation of effective interdisciplinary teamwork methods at various hierarchical levels.** • **Effective use of information sources, as well as communication and professional-assisted training resources in both mother tongue and English.**

7. Objectives of the discipline (outcome of the acquired competencies)

7.1 General objective of the discipline	• The students should acquire basic knowledge about numerical methods used in atomic physics. • The students should acquire basis skills in using high-performance computing infrastructure.
7.2 Specific objective of the discipline	• The students should become familiar with the approximation methods used in atomic physics and other fields, such as the variational method, the stationery and time dependent perturbational methods. • The students should become familiar with the ab initio methods used for the direct numerical solution of the time independent and time dependent Schrödinger equation. • The students should form their skills for programming the applications of these methods. • They should be able to solve problems and perform numerical calculations by computer individually • •The student should be able use efficient parallelization techniques to solve numerically model, which are frequently used in atomic physics.

8. Content

8.1 Course	Teaching methods	Remarks
1. Introduction. Approximation methods in atomic physics. The calculation of 2-electron matrix elements	Explication, problematization, multimedia projection, computer exemplification.	
2. Multielectron atoms. Independent electron appoximation. The coupling of angular momenta		
3. Electrostatic corrections to the Hartree-Fock method. The dependence of the energy on the total spin and on the total angular momentum.		
4. Beyond the independent electron approximation. The configuration interaction method		
5. Time dependent perturbation theory. Transition probabilities.		
6. Atomic collisions. Cross sections. The perturbational treatment of one-electron transitions		
7. The treatment of the two-electron transitions.		
8. Transitions induced by the electromagnetic field. Optical transitions. The dipole approximation.		
9. Numerical solution of the one dimensional Schrödinger equation.		
10. Numerical solution of the 3D stationary Schrödinger equation. Spatial discretization methods.		
11. Numerical solution of the time-dependent Schrödinger equation. Temporal discretization methods.		
12. Initialization and the calculation of physical quantities.		

Bibliography

1. Bransden and Joachain, The physics of atoms and molecules, Editura Tehnică, Bucureşti, 1998.
2. L. Nagy, Numerikus es kozelito modszerek az atomfizikaban (Numerical and approximate methods in atomic physics), Scientia Cluj, 2002
3. L. Nagy, Two-electron processes in fast collisions with charged particles, Nucl. Instr. Meth. B, 124 (1997), 271-280.
4. L. Nagy, Multi-electron processes in atomic collisions – Theory, Nucl. Instr. Meth B154 (1999) 23-130.
5. L. Ixaru, Metode numerice pentru ecuatii diferentiale cu aplicatii, Ed. Academiei, Bucuresti, 1979
6. T. Beu, Calcul numeric in C, Ed. Albastra, Cluj, 2000
7. Haken and Wolf, The physics of atoms and quanta, Springer Verlag, 1994
8. C. J. Joachainm N. J. Kylstra, R. M. Potvliege, Atoms in Intense Laser Fields, Cambridge University Press, 2012.

8.2 Laboratory	Teaching methods	Remarks
1. Tutorial on the use of computational clusters. Login, software selection/compilation, job submission and management. Parallelization paradigms.	Multimedia presentations followed by hands on exercises.	

2. Introduction into MPI parallelization.	Individual programing tasks.	
3. Advanced features of MPI parallelization		
4. Implementation of basic numerical methods using MPI parallelization.		
5. The PETSC MPI parallel linear algebra package.		
6. The Slepc MPI parallel eigensolver package		
7. The use of PETSC and Slepc packages for the implementation of the numerical methods used for the solution of Schrödinger equation.		
In the second part: each student receives an individual set of problem to solve (one related to the approximate methods and one related to the direct solution of the Schrödinger equation). He/she studies the theoretical background, performs the analytical calculations, writes the computer code for the numerical part and elaborates a report on the studied problems. The presentation should follow the structure of a scientific paper.		

9. Corroborating the content of the discipline with the expectations of the epistemic community, professional associations and representative employers within the field of the program

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10. Evaluation

Type of activity	10.1 Evaluation criteria	10.2 Evaluation methods	10.3 Share in the grade (%)
10.4 Course	Knowlidge, understanding and capacity of application of numerical methods in atomic physics	Oral exam	50
10.5 Seminar/lab activities	Individual work	Written report	50
10.6 Minimum performance standards			
55%			

Date ..26.06.2023………..

Signature of course coordinator ....

Signature of seminar coordinator ....

Date of approval ....

Signature of the head of department ....…............................